# Radiative correction to x-ray scattering and its relevance in condensed-matter experiments

C. Rocchi and F. Sacchetti
*Dipartimento di Fisica, Università di Perugia, Perugia 06100, Italy*
(Received 9 November 1992)

The radiative correction to the elastic scattering (Rayleigh) of a photon is calculated considering applications to high-precision condensed-matter experiments. It is found that the radiative correction can be appreciable when the incoming photon energy exceeds 1000 keV and the experimental accuracy is better than 0.1%.

The study of condensed matter using x rays is so well established that the number of applications is exceedingly large. In previous papers[1,2] the use of x-ray scattering has been considered in condensed-matter physics, with special emphasis on the proper relationship between the cross section and relevant observables. As is well known, there are two obvious applications of x-ray scattering that have a special impact on basic solid-state physics. These are the electron-density (Rayleigh scattering) and momentum-density (Compton scattering) measurements in crystals. In recent years it has been realized that the use of photon energies in the standard x-ray range, i.e., from 10 to 20 keV, is extremely limiting for the correct determination of these quantities. In fact in the case of electron-density measurements the anomalous scattering contributions contribute an appreciable fraction of the total scattering amplitude, so that one has to rely on more or less accurate calculations. Moreover, experimental problems, e.g., extinction, are more severe in the x-ray energy range. In the case of Compton scattering one has to use the impulse approximation,[3] which becomes better and better as the photon energy is increased. Therefore, in both cases the use of hard x-rays, i.e., from 100 to 1000 keV and above, can allow for a safe determination of both number and momentum densities, if one neglects the fact that this high energy is far from being negligible as compared to the rest energy of the electron. In Ref. 2 the effect of considering the relativistic correction to the x-ray cross section, both elastic and inelastic, has been discussed. However, as already observed in Ref. 2, one has also to consider the fact that the coupling constant between electron and photon, namely, the fine-structure constant $\alpha = e^2/\hbar c \simeq \frac{1}{137}$, is not a very small parameter, so that the lowest-order interpretation of the experimental cross section is expected to be good at about 1%. Recently it has been shown[4,5] that it is possible to perform elastic (Rayleigh) photon-scattering experiments at relatively high energy, with an accuracy largely exceeding 1%, so that the corrections to the cross section might become important.

In the case of Compton scattering it is now common practice to use relatively high energy and it has been recognized a long time ago[5] that higher-order corrections can play some role. In particular it is evident[2] that the correction to the Compton scattering is not negligible and *must* be considered in analyzing the experimental data.

Because of the above discussion and the fact that the rough estimate of the third-order (radiative) correction to the elastic cross section reported in Ref. 2 suggests an effect of the order of a fraction of percent, considering the possibility of performing very accurate experiments, we calculated such a correction, having in mind the application to the photon scattering off a many-electron system. To perform the calculation we followed the nonrelativistic approach presented by Heitler,[6] as a many-body relativistic theory presents some difficulty.[7] This procedure is somewhat contradictory because the radiative correction is expected to be relevant at high photon energy, so that a nonrelativistic approach could be considered doubtful. However, this procedure, when applied to the Compton scattering from a single free electron, provides the same result as the fully relativistic theory,[8] so that one can be confident that the approach is valid.

According to this discussion we split the total Hamiltonian into three contributions:

$$H = H_e + H_{\rm rad} + H_{\rm int} , \tag{1}$$

where $H_e$ is the electron Hamiltonian in the absence of the field, $H_{\rm rad}$ is the free radiation Hamiltonian, and $H_{\rm int}$ represents the interaction between electron and field. In the nonrelativistic limit $H_{\rm int}$ can be written as

$$H = H^{(1)} + H^{(2)} = -\frac{e}{2mc}\sum_i [\mathbf{p}_i \cdot \mathbf{A}(\mathbf{x}_i) + \mathbf{A}(\mathbf{x}_i)\cdot \mathbf{p}_i] + \frac{e^2}{mc^2}\sum_i A^2(\mathbf{x}_i) , \tag{2}$$

where $\mathbf{x}_i$ and $\mathbf{p}_i$ are position and momentum operators of the $i$th electron and $\mathbf{A}(\mathbf{r})$ is the vector potential operator. The elastic scattering cross section is written as

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar c}\rho_F |K_{0F}|^2 , \tag{3}$$

where $\rho_F$ is the density of final states and $K_{0F}$ is the appropriate matrix element, containing terms linear and quadratic in $\alpha$. One can write

$$K_{0F} = K_2 + K_4 , \tag{4}$$

0163-1829/93/47(22)/15283(3)/$06.00  

where $K_2$ is proportional to $\alpha$ and $K_4$ is proportional to $\alpha^2$. $K_2$ is due to first-order contributions from $H^{(2)}$ and second-order contributions from $H^{(1)}$ (anomalous scattering). This lowest-order result is extensively considered in the literature and does not need further analysis. $K_4$ contains several terms and its general form is reported in Ref. 6. To the purpose of deriving a closed-form result still employing approximations adequate for quantitative comparison to the experimental data, we proceed as follows. Considering that the radiative corrections can be nonnegligible only when the incoming photon has a high energy, one can neglect the electron momentum matrix element in the ground state as compared to the photon momentum. This approximation considerably simplifies the expression of $K_4$. At the same time all electron intermediate states can be approximated as states obtained from the $N$-electron ground state by exciting one electron only to an almost free-electron state having a well-defined momentum. This approach, already employed in Ref. 2, is particularly convenient to avoid an explicit description of the ground state. Using this procedure we performed all the sums on the intermediate states by integrating on the intermediate photon wave vectors and by summing on the relative polarizations. The calculation is very long but similar to that of Ref. 6 for Compton scattering and as in that case it contains two diverging terms. The first one, which behaves as $\ln(\hbar c k'/mc^2)$ as the intermediate photon wave vector $k'$ diverges, corresponds to charge renormalization and consequently can be disregarded. The second diverging term is due to the infrared catastrophe and deserves some care. In fact it is well known[6,8] that such a divergence disappears if one takes into account a term containing two photons in the final state, one of which has a vanishingly small energy. It is clear that the process having a very low-energy photon other than the main one is not experimentally distinguishable from a normal process with one photon only in the final state. However, one has to remember that in a scattering experiment from a crystalline solid the presence of Bragg diffraction allows for the identification of highly elastic processes so that an extremely small energy[4] is left for the additional soft photon in the final state. In particular in the limit of ideal elastic scattering no soft photon can be present in the final state and one can show that the infrared divergence disappears proportionally to the maximum allowed inelasticity. The final form for the cross section, accurate to the order $\alpha^3$ and for energy small as compared to the electron rest energy is as follows:

$$\frac{d\sigma}{d\Omega}=\tfrac{8}{3}r_0^2\frac{\alpha}{\pi}|F(Q)|^2(\mathbf{e}\cdot\mathbf{e}_0)[(\mathbf{e}_0\cdot\mathbf{k})(\mathbf{e}\cdot\mathbf{k}_0)-2(\mathbf{e}\cdot\mathbf{e}_0)]\times(\hbar c k_0/mc^2)^2\ln(\hbar c k_0/mc^2)+|F(Q)|^2(\mathbf{e}\cdot\mathbf{e}_0)^2\ , \tag{5}$$

where $\mathbf{k}_0$, $\mathbf{e}_0$, $\mathbf{k}$, and $\mathbf{e}$ are the incoming and outgoing photon wave vector ad polarization and $F(Q)$ is the atomic scattering factor:

$$F(Q)=\int_{\mathrm{WS}} n(\mathbf{r})\exp[i\mathbf{Q}\cdot\mathbf{r}]d\mathbf{r}\ , \tag{6}$$

the integral being performed over the Wigner-Seitz cell and $n(\mathbf{r})$ being the electron number density in the ground state. It is interesting to observe that both terms of the cross section contain the scattering factor in the same way, so that the well-known behavior of the cross section is not affected by the radiative correction.

To identify the relevance of the correction we have derived, the energy dependence of the ratio between the scattering amplitude due to the correction and the lowest-order term at zero scattering angle is reported in Fig. 1. Actually an elastic process at zero angle is clearly meaningless. Nevertheless it is useful to study this particular condition because the elastic scattering at high energy is confined to a small angle and the angular dependence of the cross section is weak apart from that due to the scattering factor. Of course one cannot establish a proper energy range where Eq. (5) holds; however, one can easily find that at zero scattering angle the ratio between $\alpha^3$ and $\alpha^2$ terms in Eq. (5) is exactly the same as that obtained in Ref. 6 for Compton scattering in a limit similar to the present one. This behavior confirms a guess used in Ref. 2 to roughly evaluate the radiative correction. Therefore, considering that, on increasing the energy, the angular range where the elastic scattering is appreciable decreases, it is quite reasonable to calculate the radiative correction at any incoming energy confining the calculation to the low angle, where there is identification between Compton and Rayleigh processes. Following the above discussion, we used the result deduced in Ref. 8 for Compton scattering to determine the ratio between $\alpha^2$ and $\alpha$ contributions to the scattering amplitude at zero scattering angle. A closer examination of the kinematics of the elastic scattering allows us also to establish that the identification of Rayleigh and Compton matrix elements is meaningful at any scattering angle if one adapts the four-momentum invariance at the scattering event and assumes the same energy for both incoming and outgoing photons. According to the previous discussion about the infrared catastrophe, we neglected all the contributions due to the additional soft photon in the final state. To give an estimate of the higher-order term at high energy we report in Fig. 1 also the fully rela-

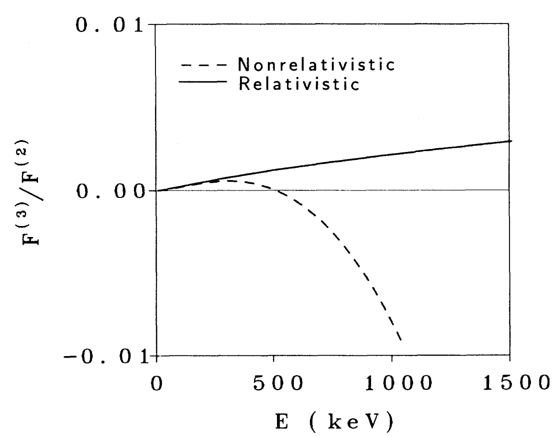


FIG. 1. Energy dependence of the ratio between $\alpha^2$ ($F^{(3)}$) and $\alpha$ ($F^{(2)}$) contributions to the scattering amplitude. Solid line, fully relativistic calculation; dashed line, nonrelativistic approximation.

tivistic result. As we can see the nonrelativistic calculation is good up to 100 keV, while the fully relativistic calculation shows a rather monotonous trend. Although the correction to the Rayleigh scattering amplitude is small, we see that it can be experimentally observed when the photon energy is higher than 1000 keV and the experimental accuracy 0.1% or better. Actually such an experiment devoted to the measurement of the radiative correction is within the best experimental possibilities,[4,5] so that a properly performed study could establish the validity of the results reported in Fig. 1. The data already available[5] at 1381 keV are in reasonable agreement with present estimate, but a larger energy range should be studied to give a definitive answer.

As a conclusion we can say that the radiative correction has a small but nonnegligible relevance in very accurate condensed-matter experiments, but in view of the basic role of such a correction for quantum theory of radiation, an experiment devoted to this matter would be extremely important.

[1]F. Sacchetti, J. Phys. F **11**, 511 (1981).
[2]F. Sacchetti, Phys. Rev. B **36**, 3147 (1987).
[3]M. J. Cooper, Rep. Prog. Phys. **48**, 415 (1985).
[4]E. G. Kessler *et al.*, J. Phys. G Suppl. **14**, 167 (1988).
[5]S. Deway *et al.* (unpublished).
[6]W. Heitler, *The Quantum Theory of Radiation* (Oxford University Press, Oxford, 1954), p. 327.
[7]J. Sucher, Phys. Rev. A **22**, 348 (1980).
[8]L. M. Brown and R. P. Feynman, Phys. Rev. **85**, 231 (1952).